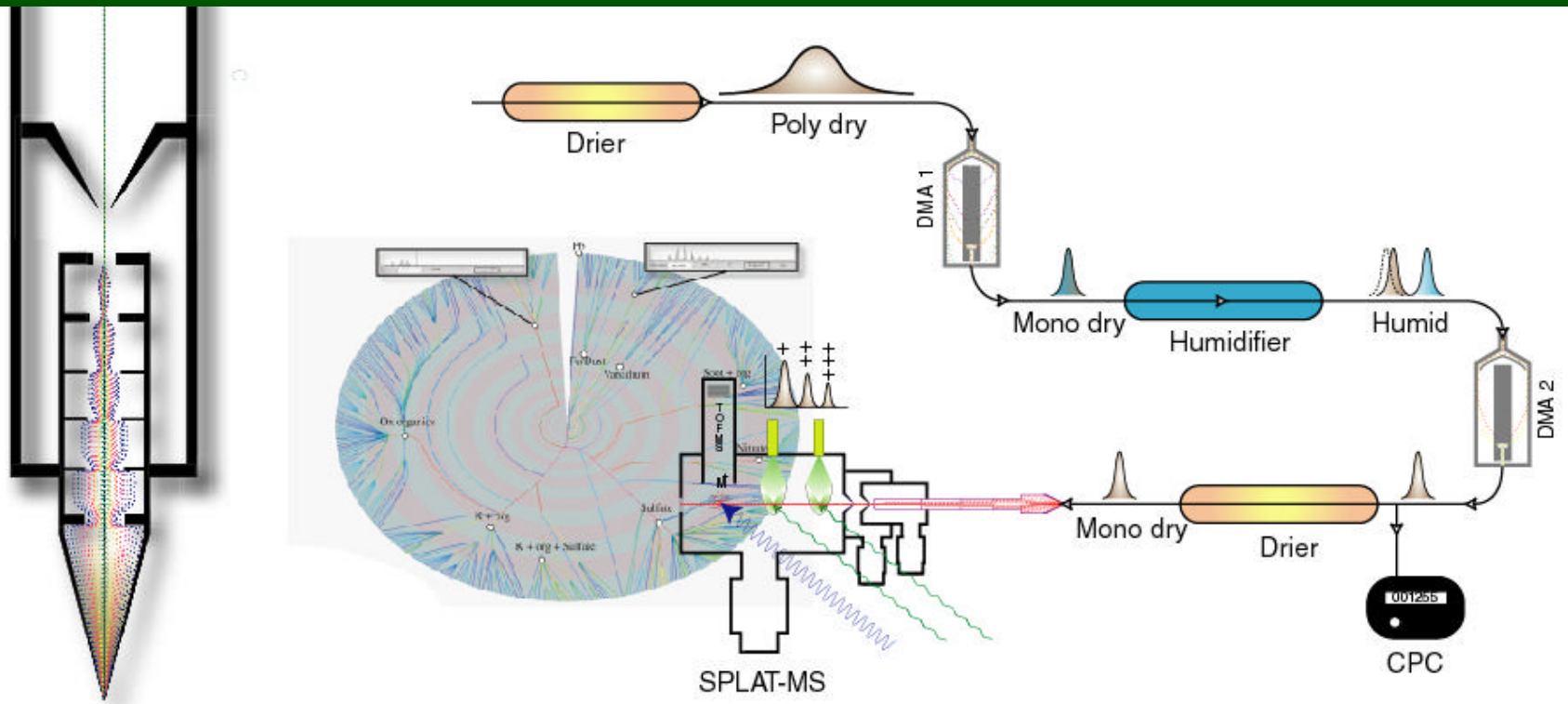
SPLAT-MS: Single Particle Laser Ablation Time-of-flight Mass Spectrometer



Alla Imre and Dan Imre

AKNOLEDGMENTS

Jian Wang	BNL	Klaus Muller	SUNYSB
Gunner Senum	BNL	Peter Imrich	SUNYSB
Jeong-Ho Han	BNL	Wei Zhu	SUNYSB
Logan Chieffo	SHU	Ray Mugno	SUNYSB
Tim Onasch	BNL		
Susan Oatis	SHU	Paul O’Connor	BNL
Mike Alexander	PNNL	Jack Fried	BNL

OUTLINE

- Single particle MS basics
- SPLAT-MS performance
- SPLAT-MS beyond size and composition
- Single spore M-D characterization

- SpectraMiner data analysis and visualization
- The interactive dendogram
- Exploring particle data

Single Particle Properties Real-Time Measurements

Here today

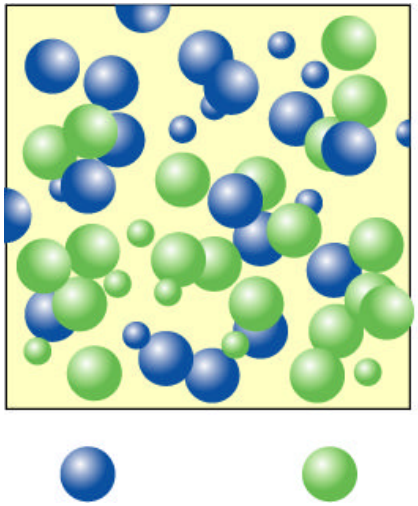
- Size
- Composition
- Density (effective density)
- Water uptake

Coming soon

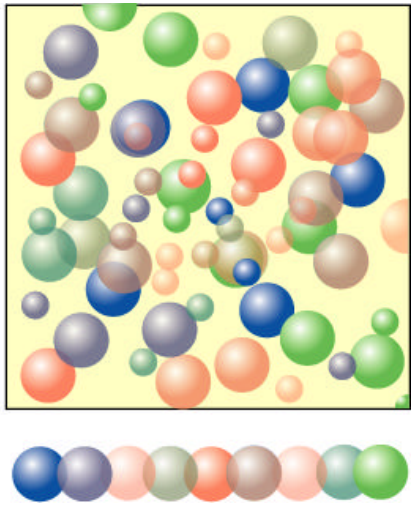
- Shape
- Optical – scattering, phase function, fluorescence
- Quantitative soot content

WHY?

Particles come internally and externally mixed

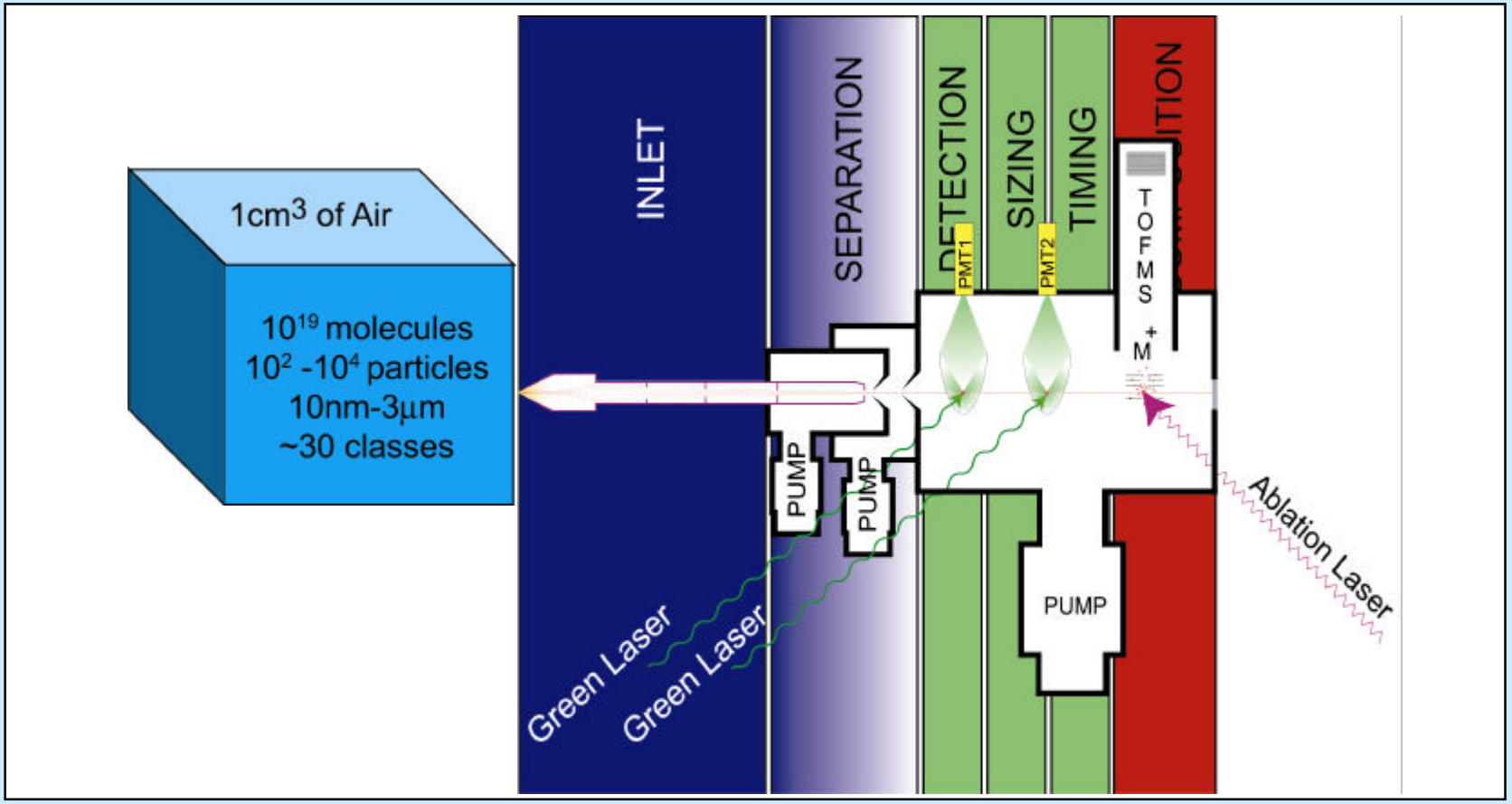


Externally mixed

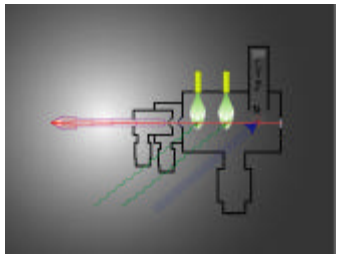


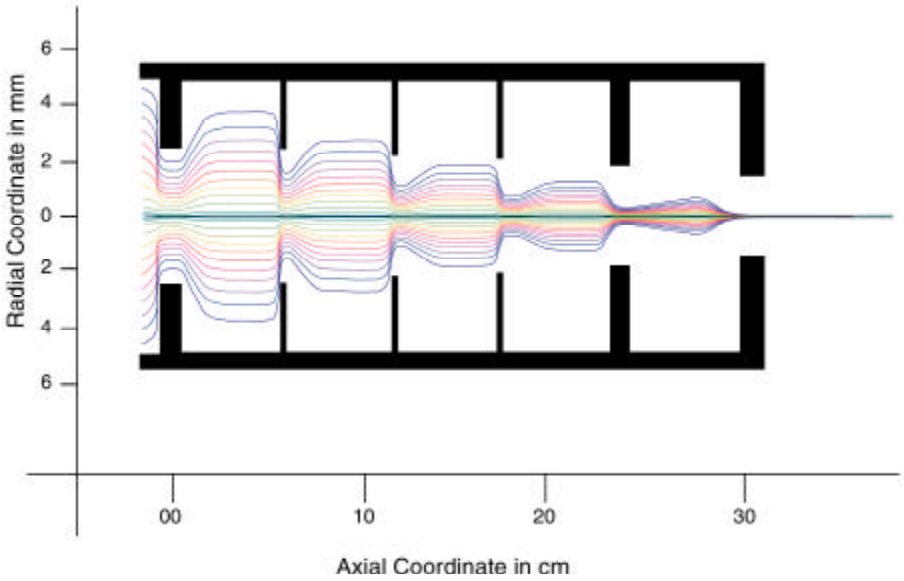
Internally mixed

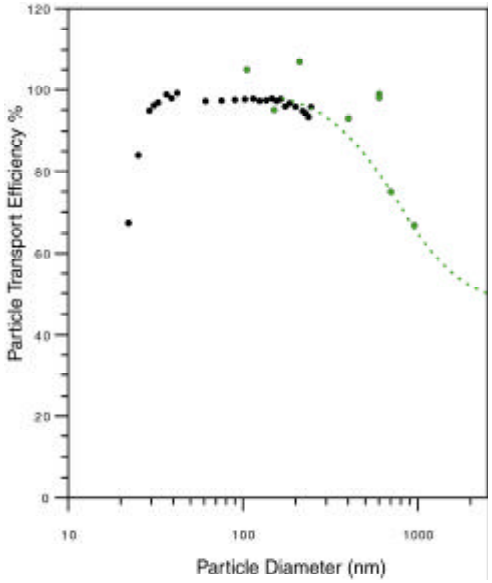
Single Particle Mass Spectrometry: Basics



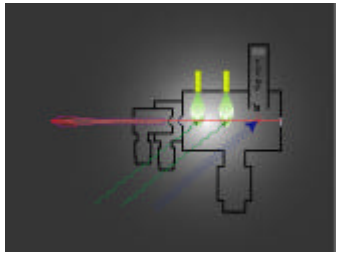
INLET

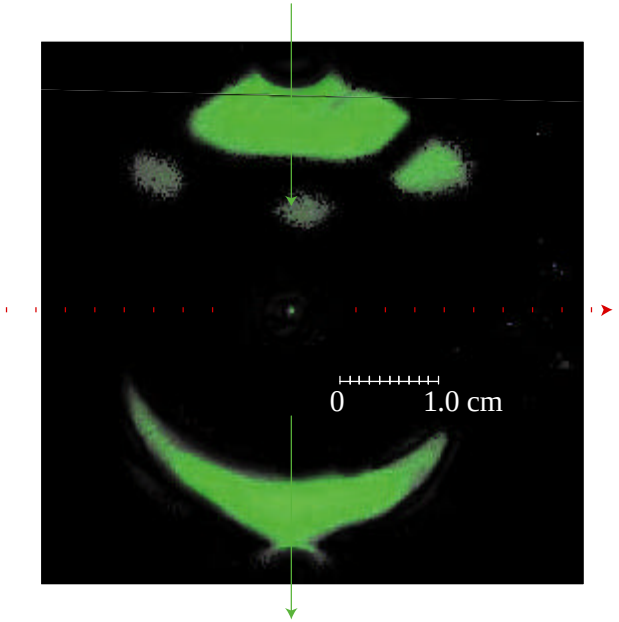



Radial Coordinate in mm
6
4
2
0
2
4
6
00
10
20
30
Axial Coordinate in cm

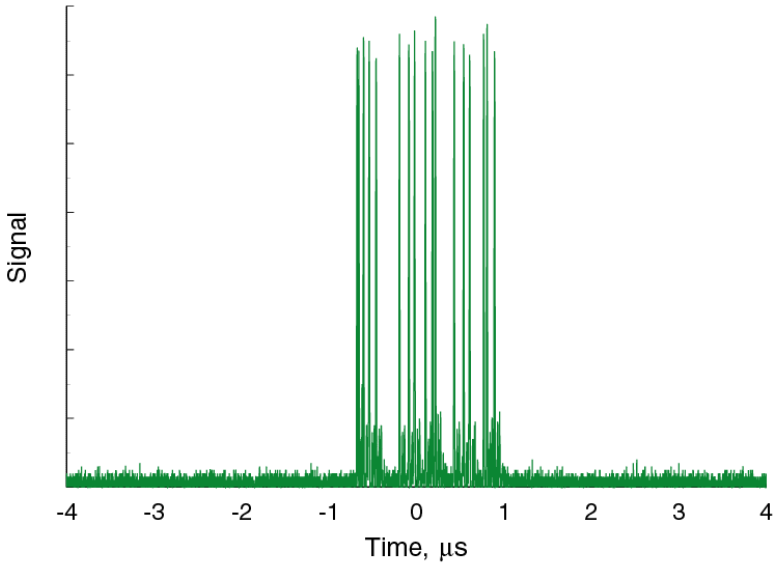

Particle Transport Efficiency %
120
100
80
60
40
20
0
10
100
1000
Particle Diameter (nm)

DETECTION

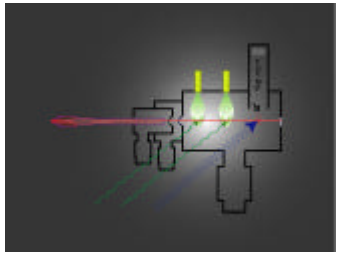


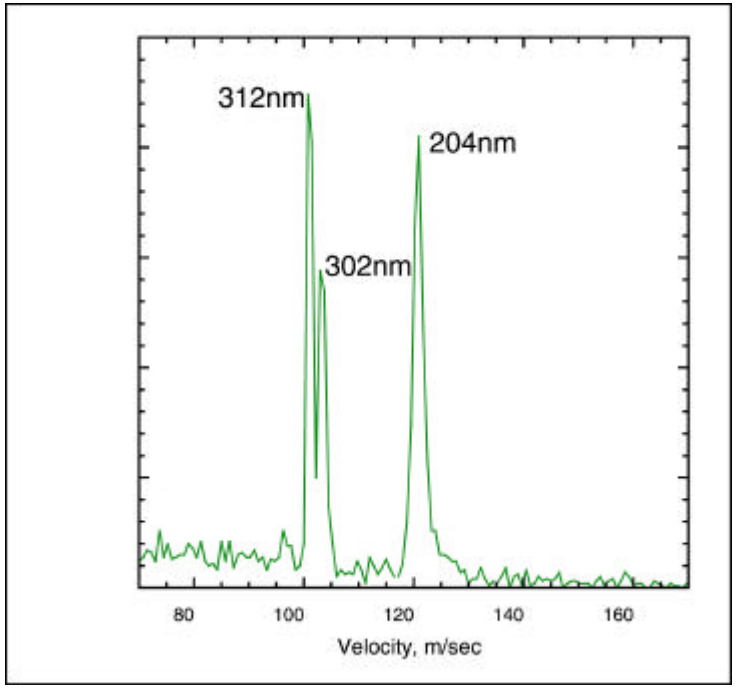


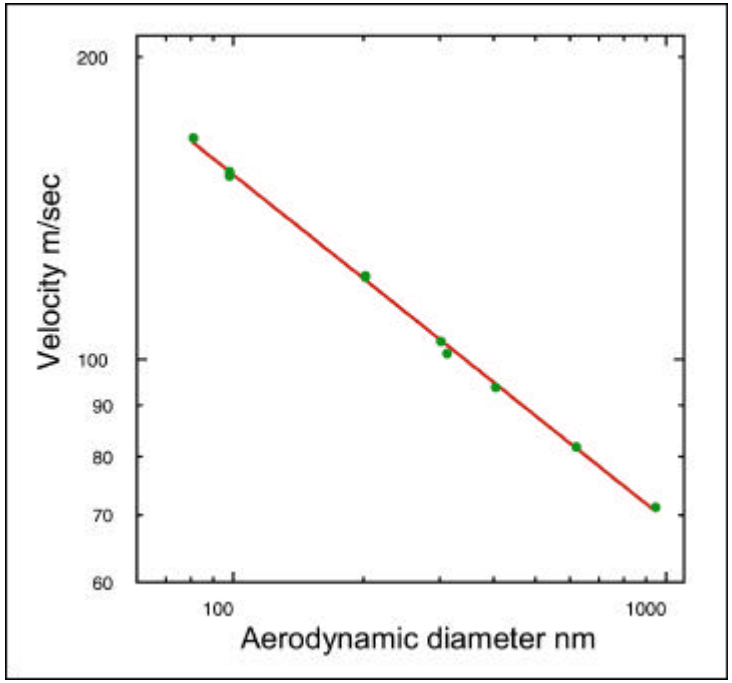
Scattered light signal from PMT, generated by 80 nm particle



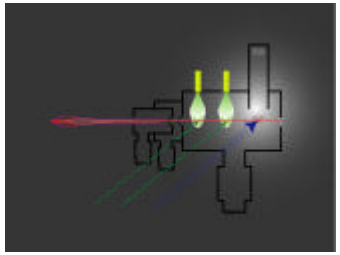
AERODYNAMIC SIZING

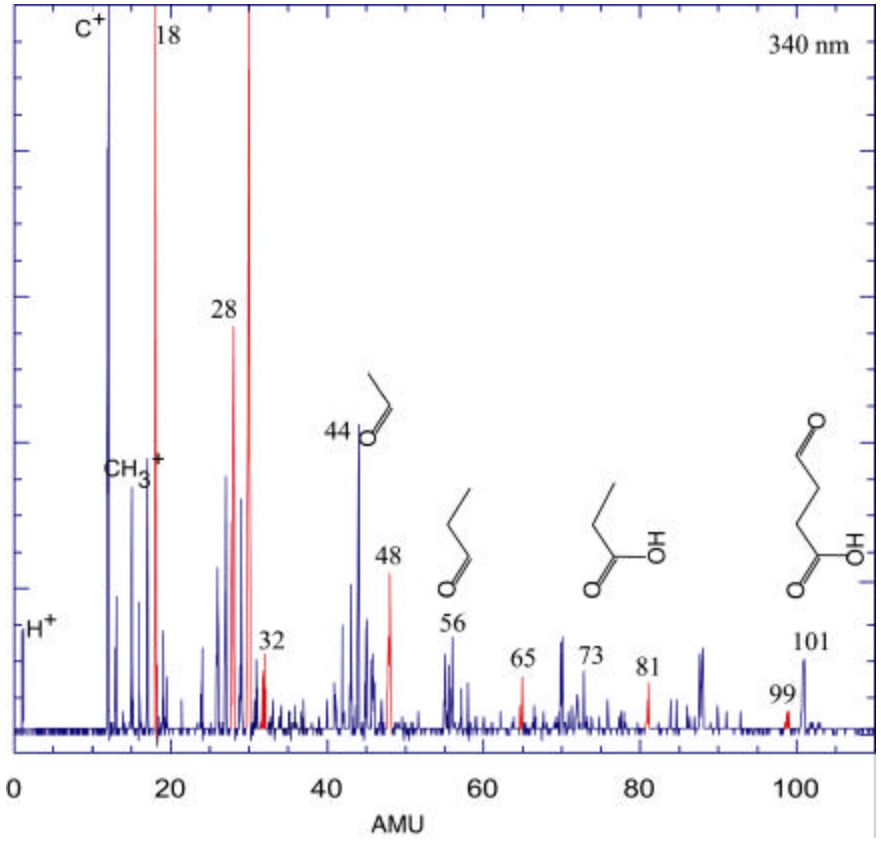




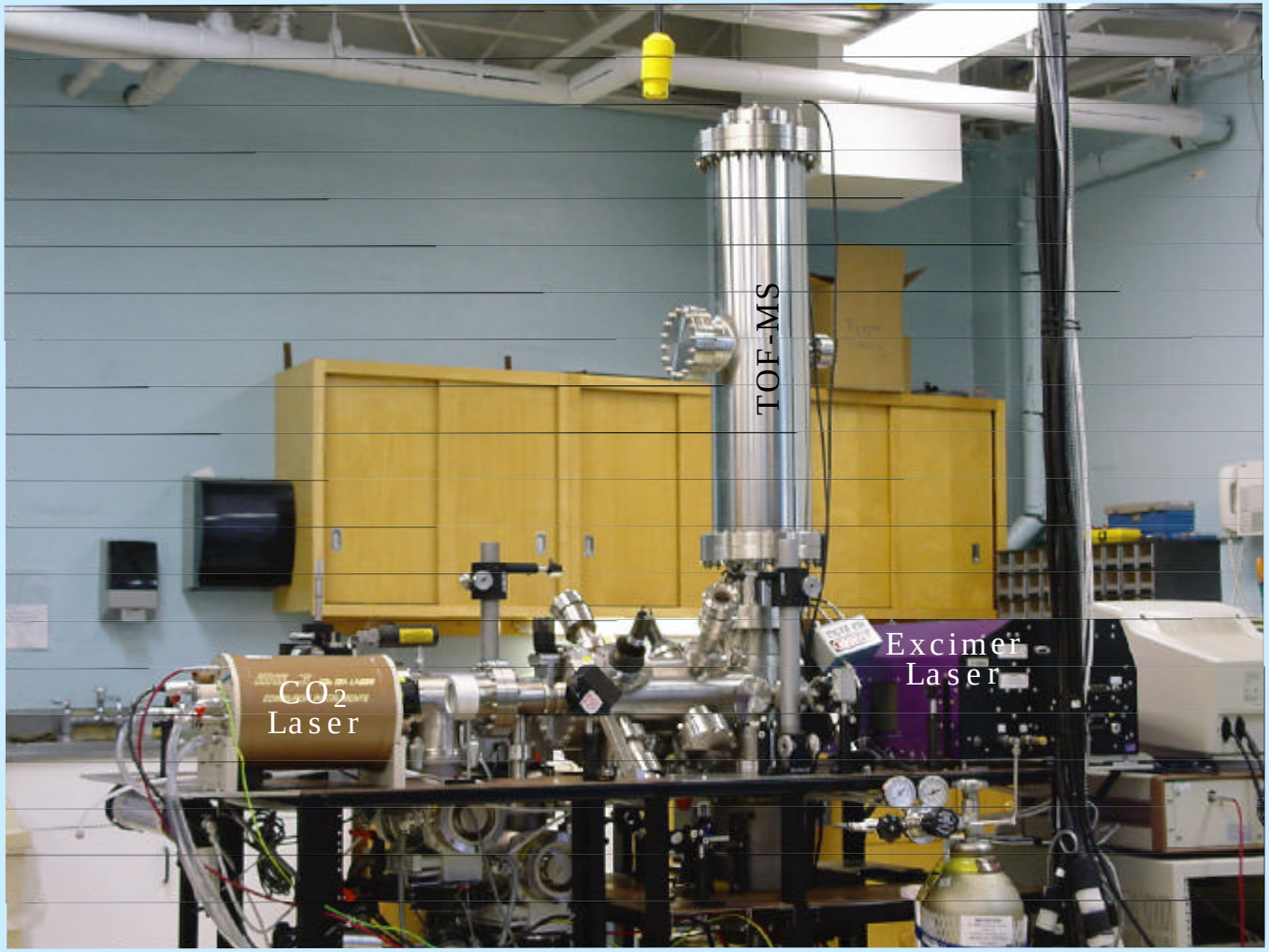


MASS SPECTRUM OF AMMONIUM SULFATE/SUCCINIC ACID PARTICLE





SPLAT-MS PHOTO



FIELD DEPLOYMENTS

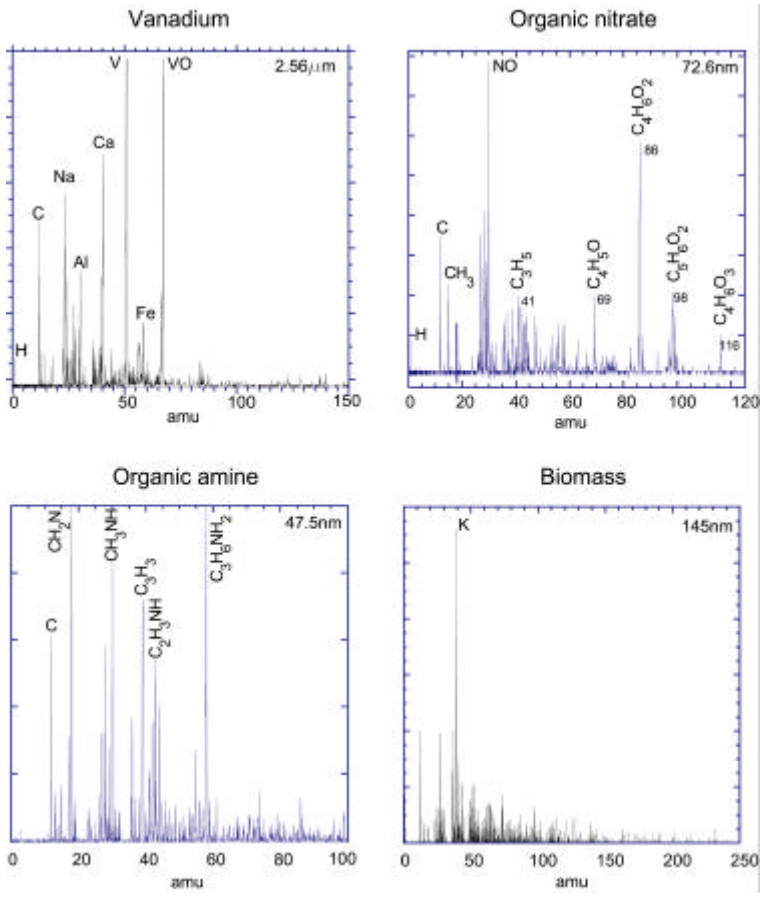
TX 2000 Air Quality Study Houston TX
August-September 2000

Aerosol Characterization Experiment Cheju
Island Korea April 2001

PM2.5 Technology Assessment and
Characterization Study, NY July 2001

Mercedes A170 Engine Characterization,
NTRC Oak Ridge TN February 2003

4 Little Atmospheric Particles



ABLATION WILL NEVER BE QUANTITATIVE

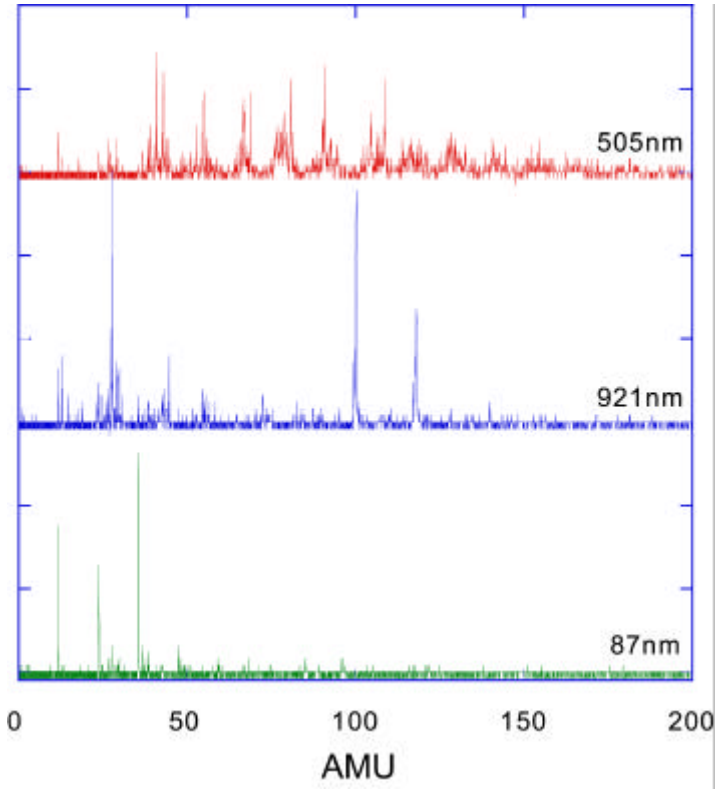
&

WE WILL NEVER IDENTIFY ORGANICS BY NAME

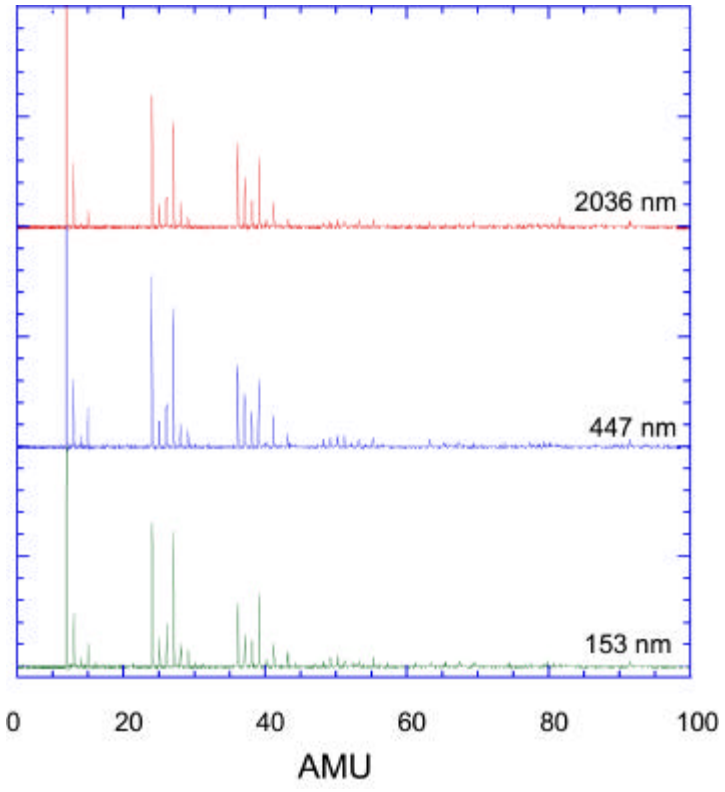
WE CAN DO BETTER

SEPARATE IONIZATION AND EVAPORATION

SEPARATION OF EVAPORATION FROM IONIZATION

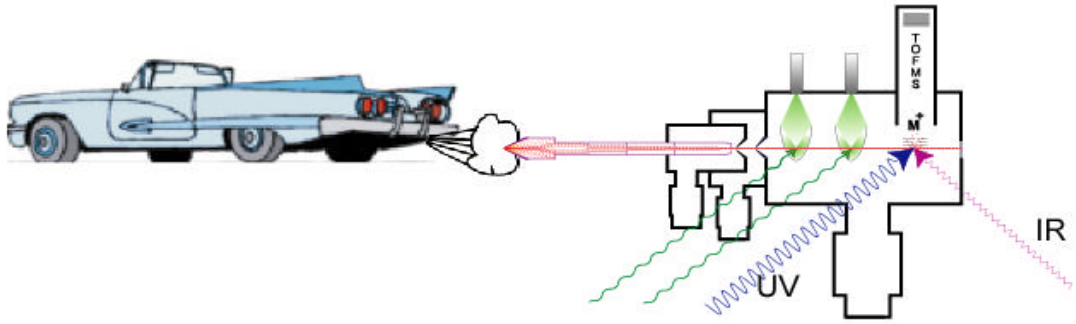


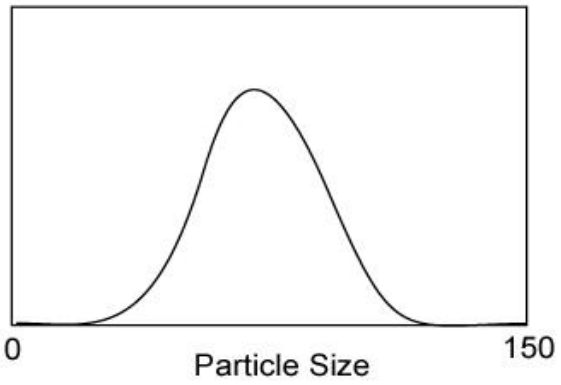
Ablation by UV laser only

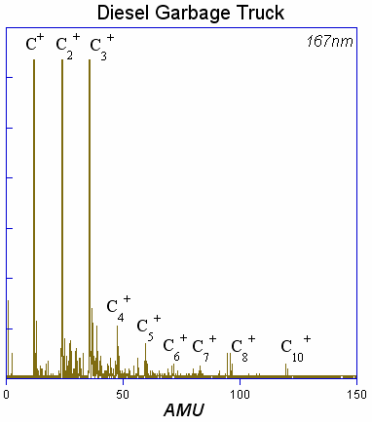


CO_2 laser evaporation UV ionization

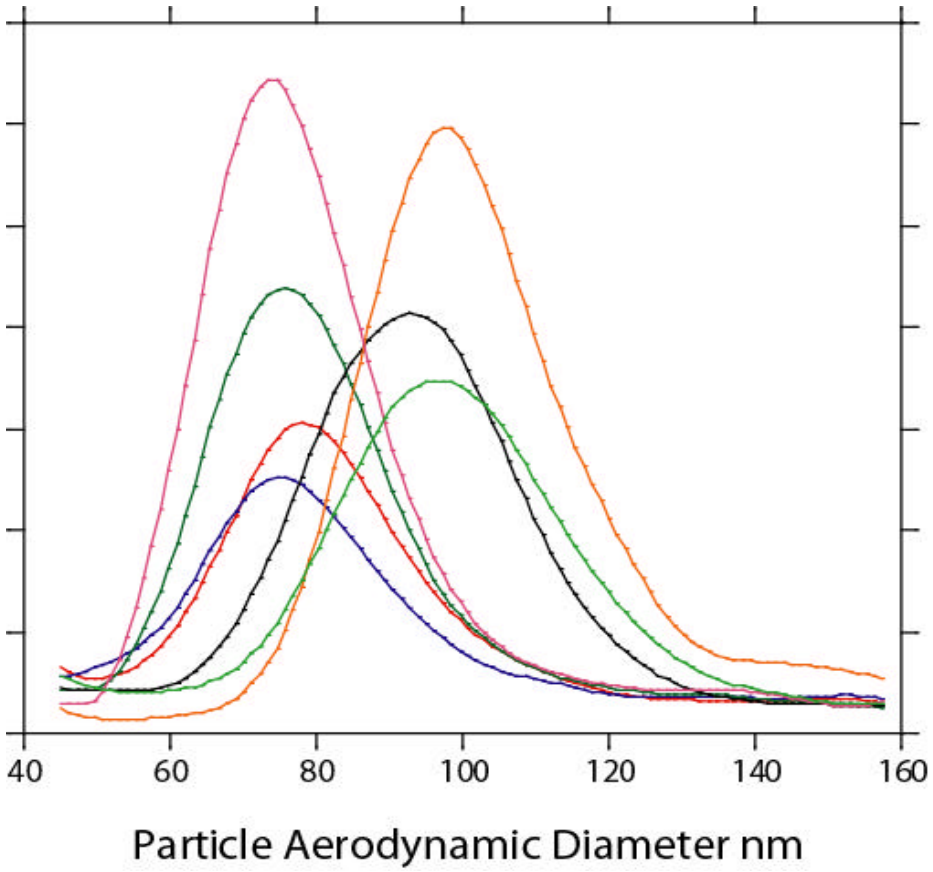
Application to Automobile Exhaust Emission





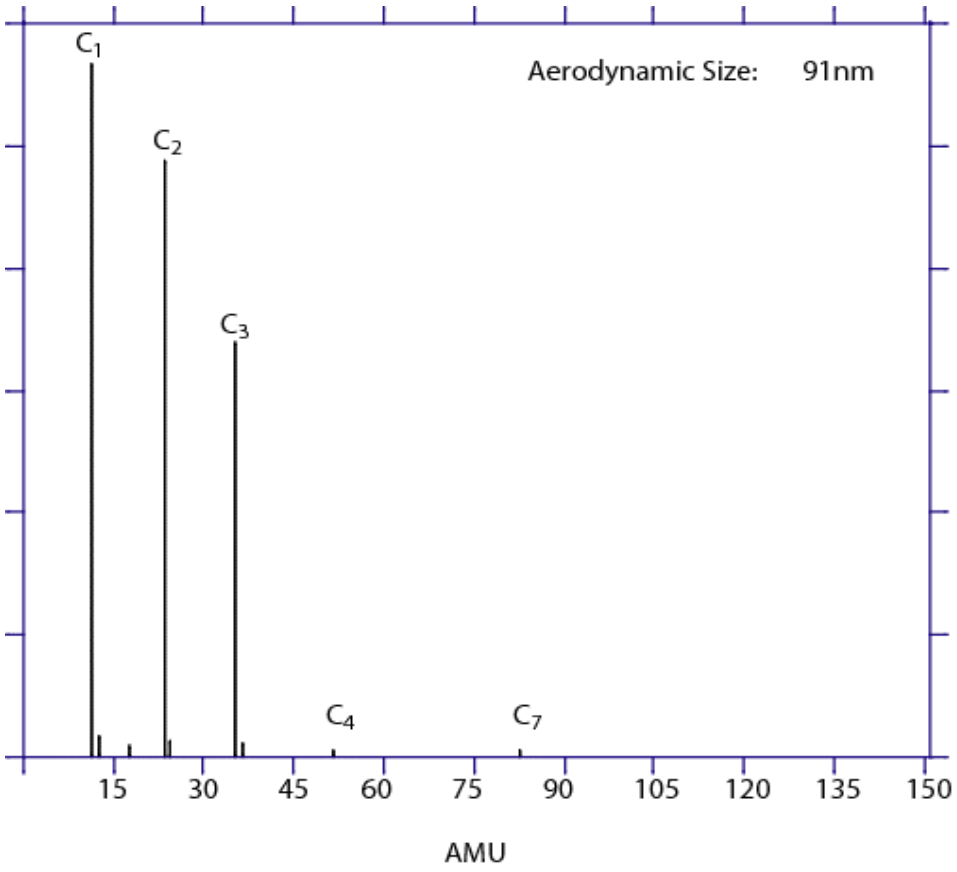


Size Distributions of Particles Observed by SPLAT-MS



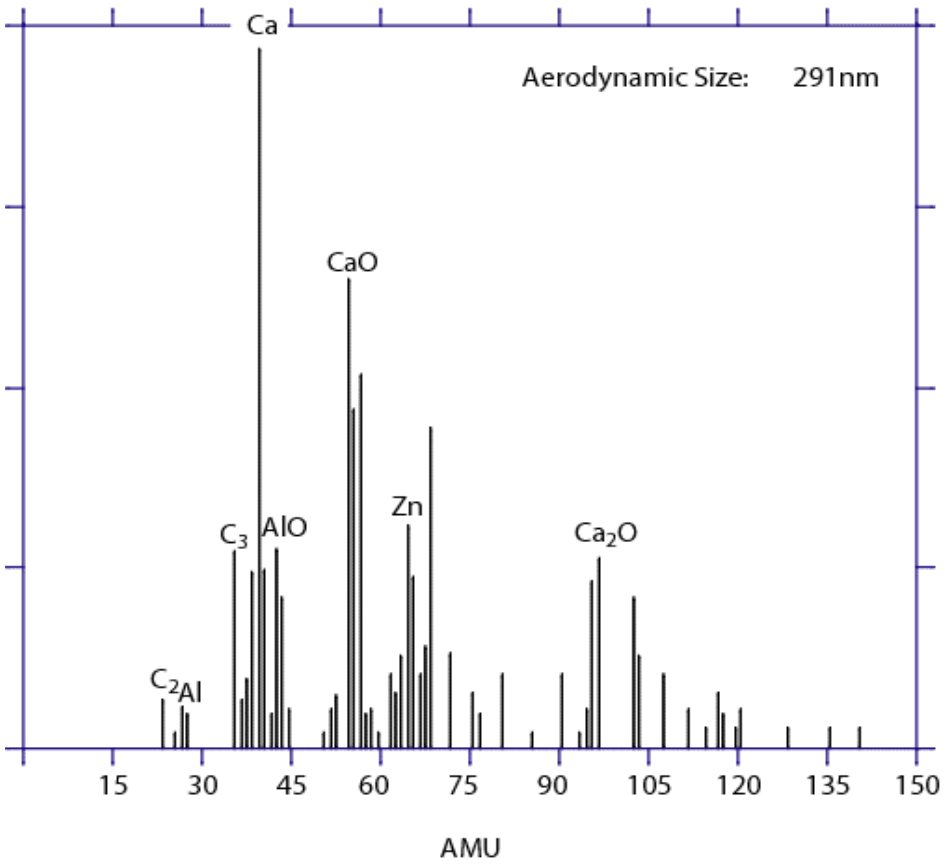
Spectra of a Few Little Exhaust Particles

SOOT



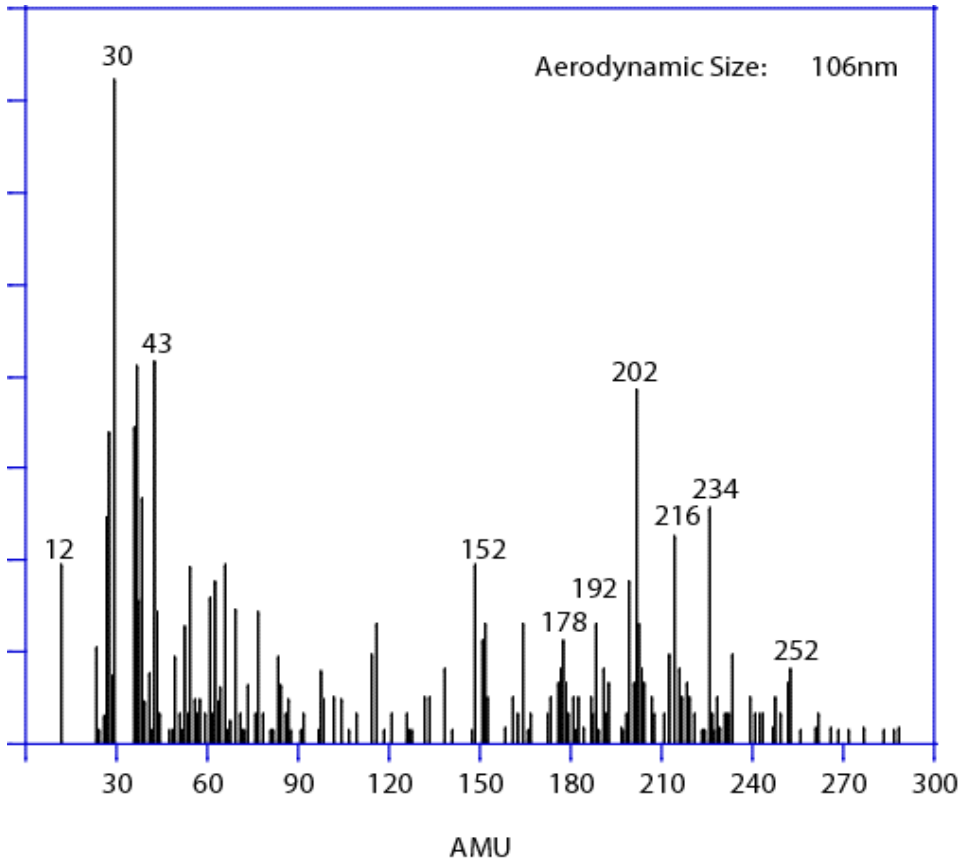
Spectra of a Few Little Exhaust Particles

Lube Additives



Spectra of a Few Little Exhaust Particles

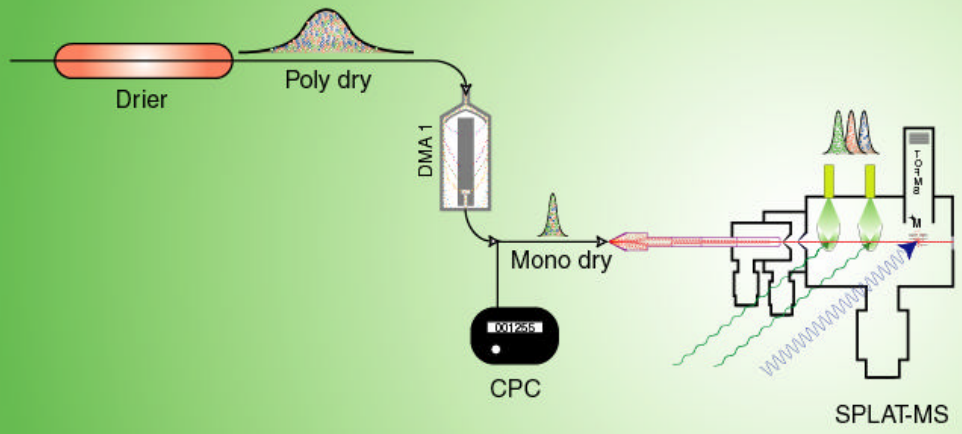
PAHs



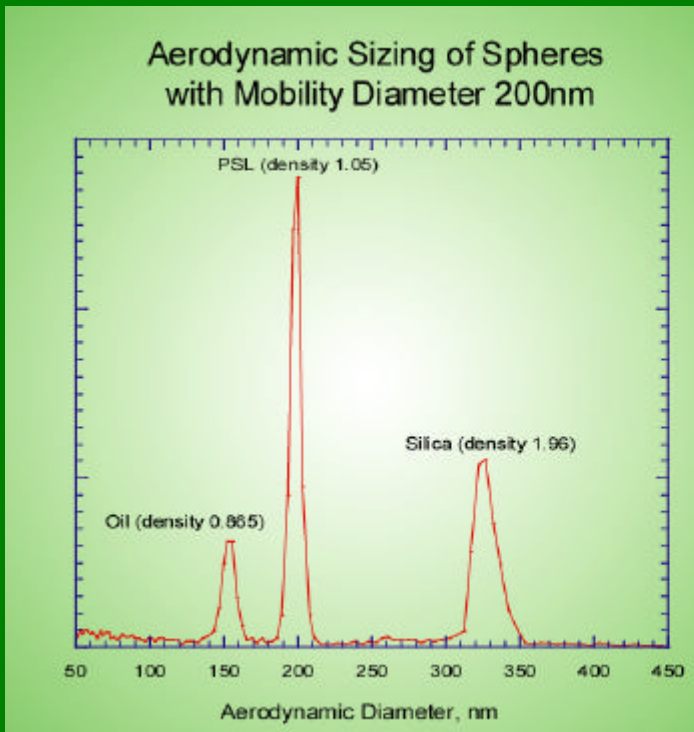
30	**NO**
152	**178-C_2H_2**
178	**phenanthrene**
192	**C_1 Alkyl phenanthrene**
202	**Pyrene**
216	**Alkyl pyrene**
234	**C_4 Alkyl phenanthrene**
252	**Benzo pyrene**

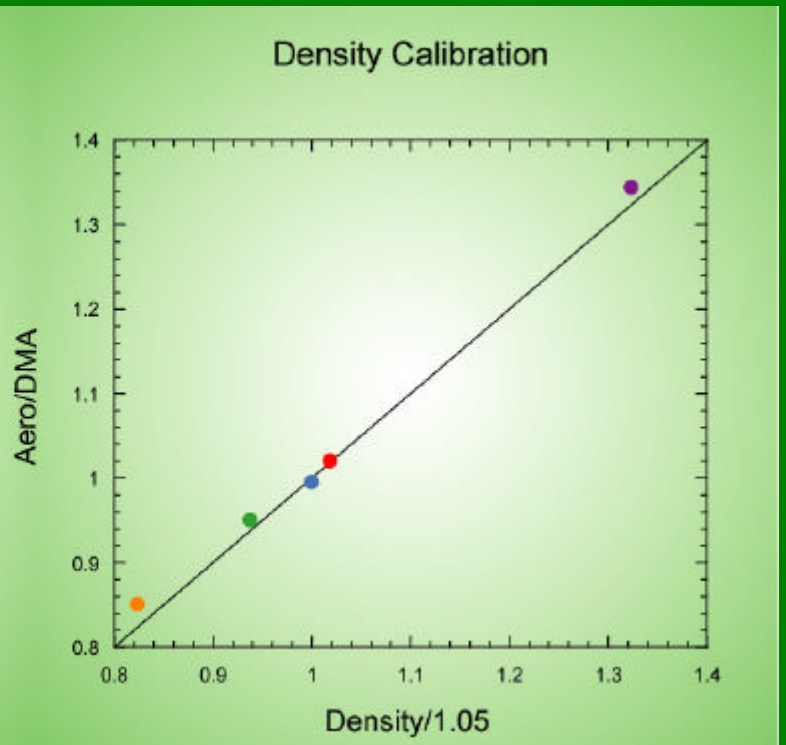
Size, Composition & Density

D_{aero}/D_{DMA}=Density



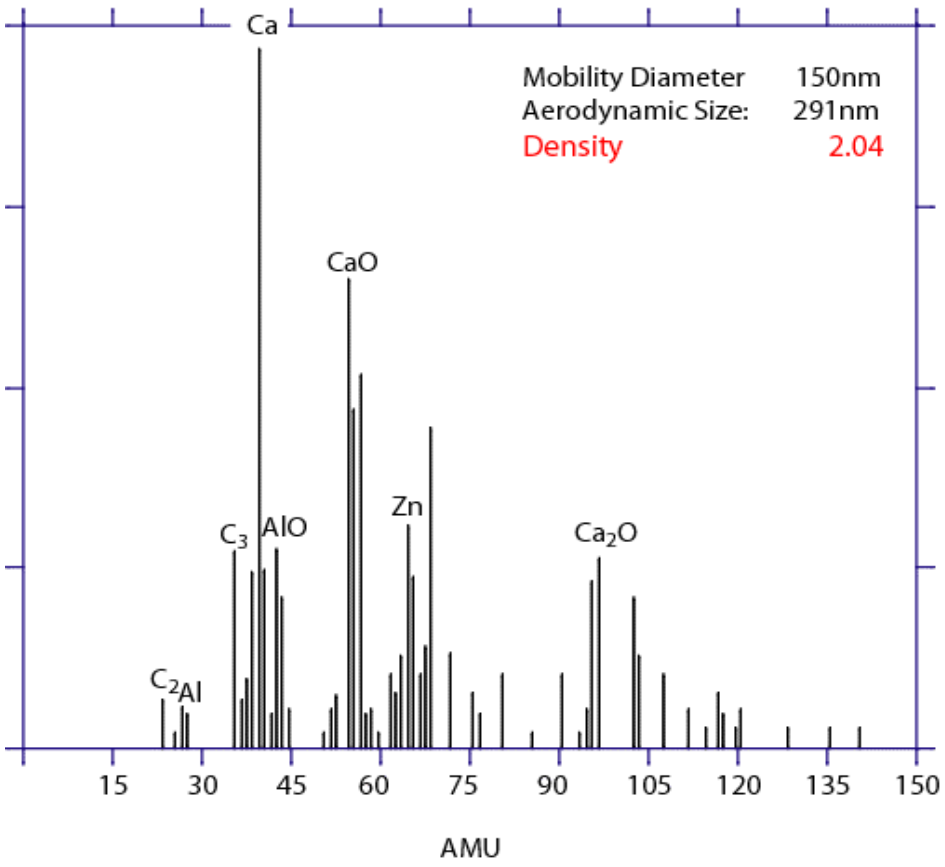
Density of 200nm Particles





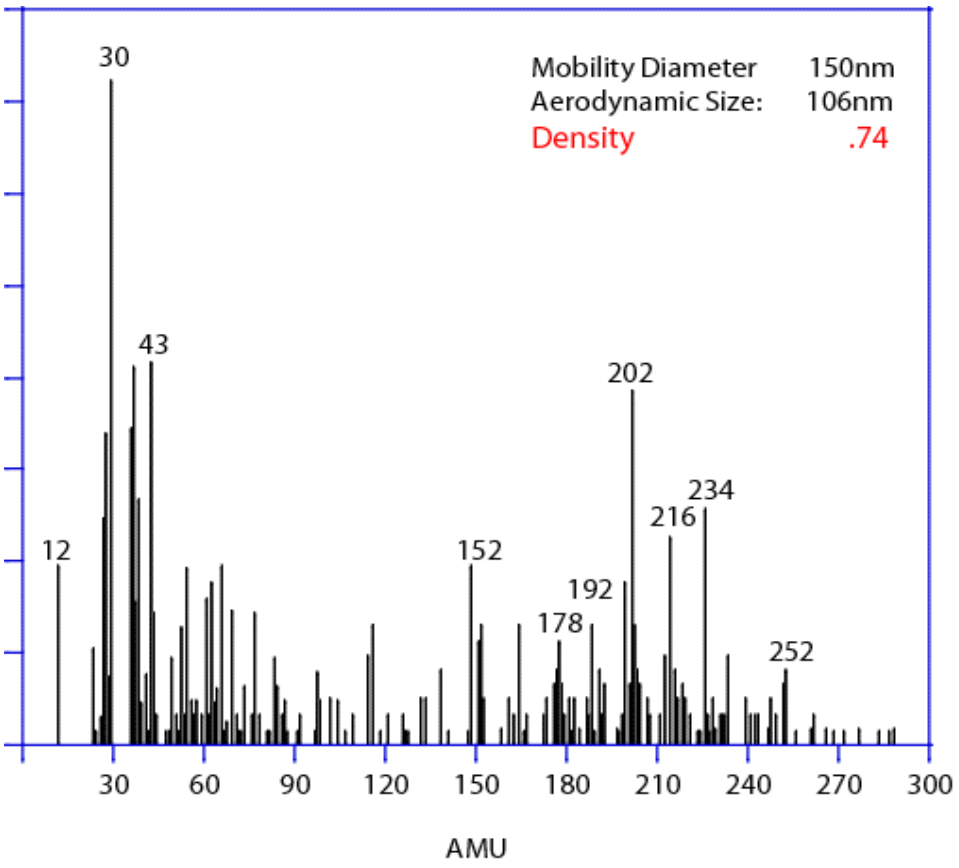
Density of the Little Exhaust Particles

Lube Additives



Density of the Little Exhaust Particles

PAHs



30	NO
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178	phenanthrene
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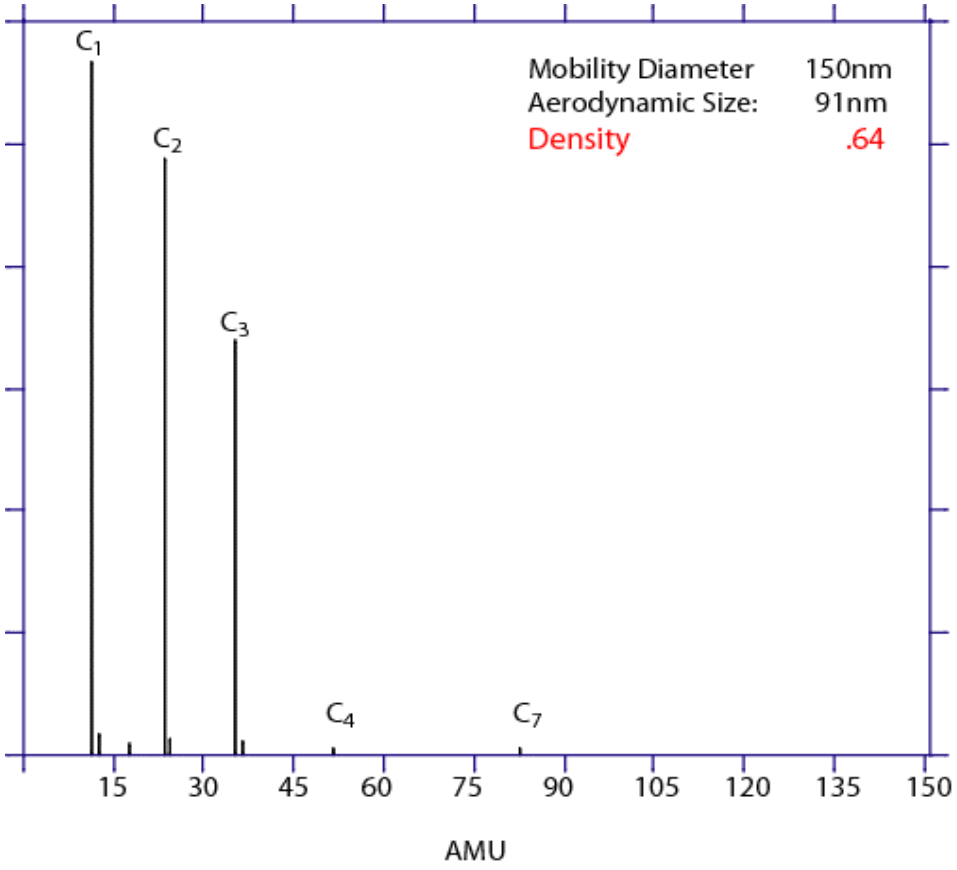
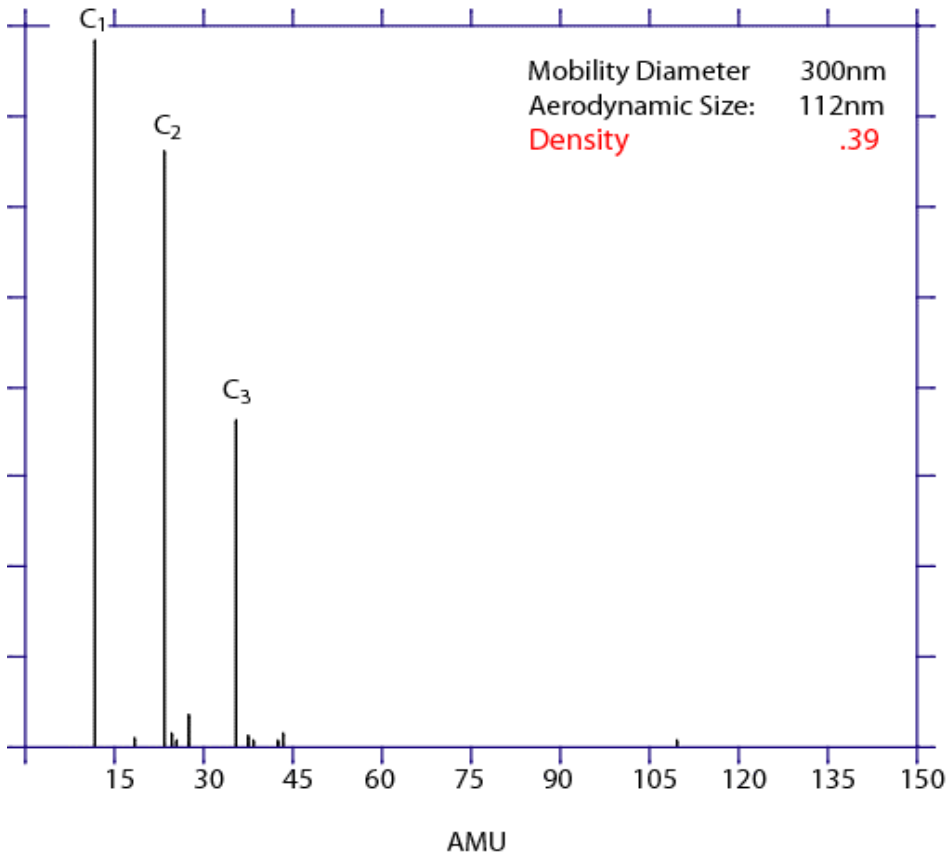
Density of the Little Exhaust Particles

SOOT

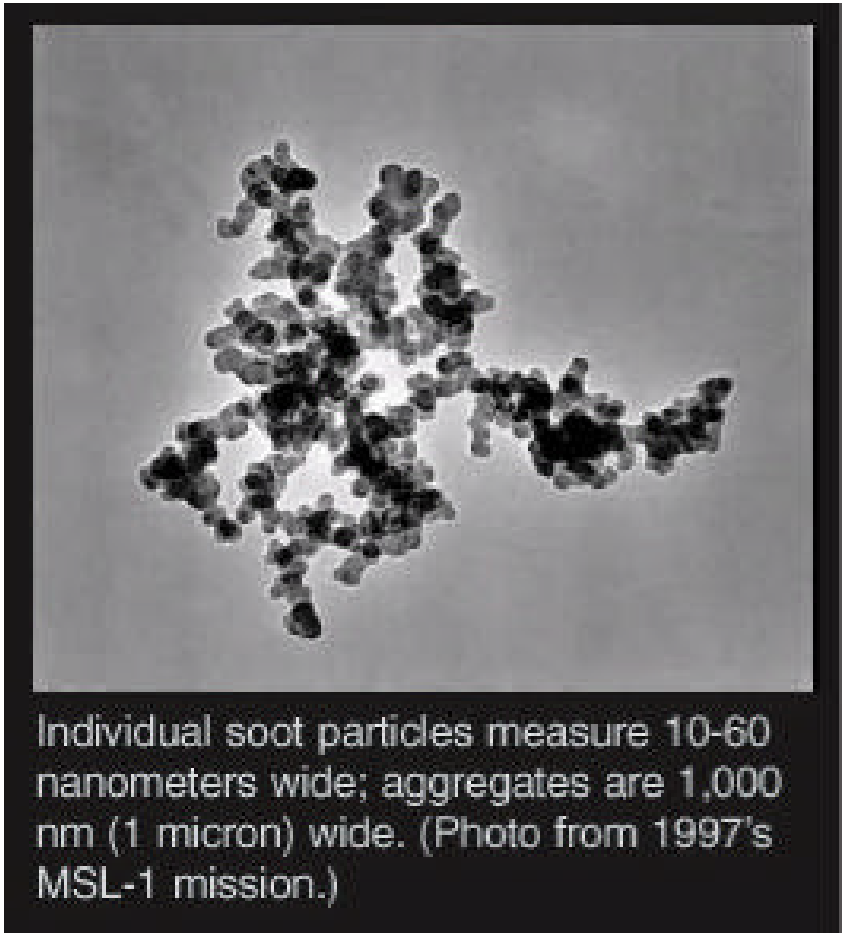


Density of the Little Exhaust Particles

SOOT

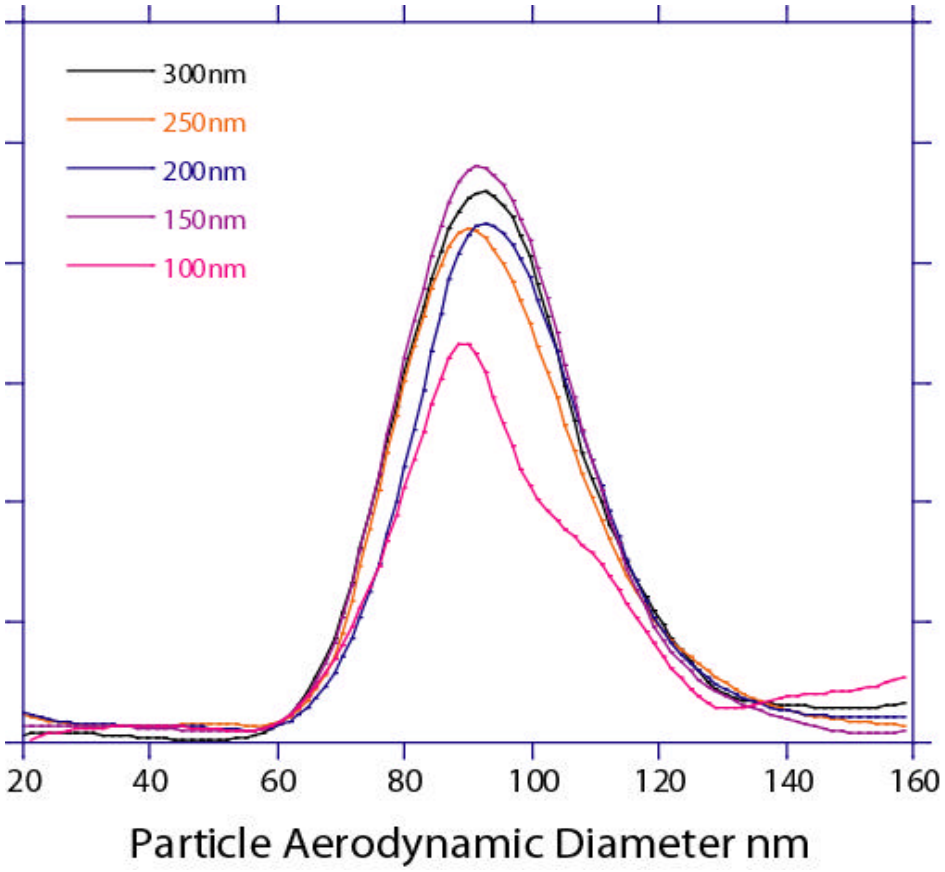


SOOT

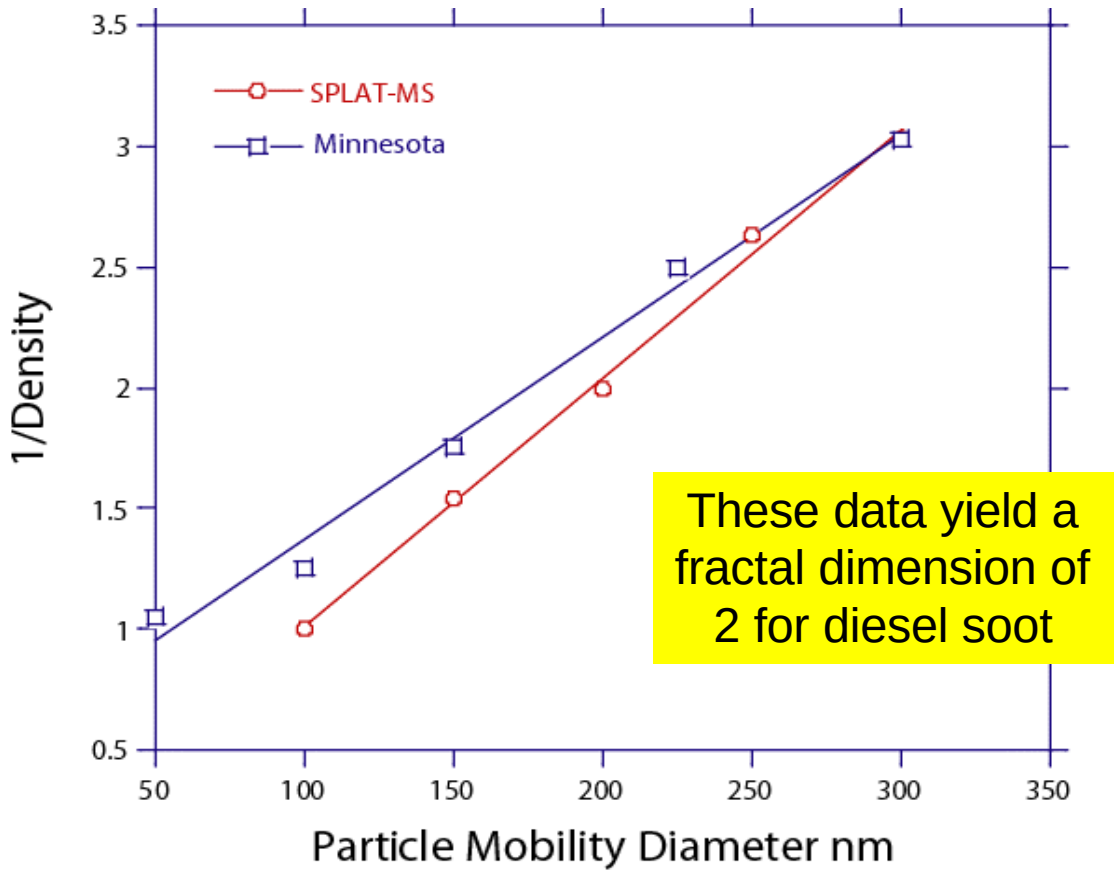


Individual soot particles measure 10-60 nanometers wide; aggregates are 1,000 nm (1 micron) wide. (Photo from 1997's MSL-1 mission.)

Size Density Relationship for Soot Particles



Size Density Relationship for Soot Particles



BIOLOGICAL WARFARE

Detection of Biological Warfare agents

requires high **sensitivity** & **selectivity**

The ultimate detection limit

SINGLE SPORE

High selectivity through

M-D characterization

SENSITIVITY REQUIREMENT

Biological Agent	***Detection Goal**
Botulinum Toxin	200 org./ cm^3 second
Yersinia Pestis	200 org./ cm^3 second
Coxiella Burnetii	200 org./ cm^3 second
Rift Valley Fever Virus	40 org./ cm^3 second
Bacillus Anthracis	40 org./ cm^3 second

*Based on a typical soldier breathing 1000 liters/hour

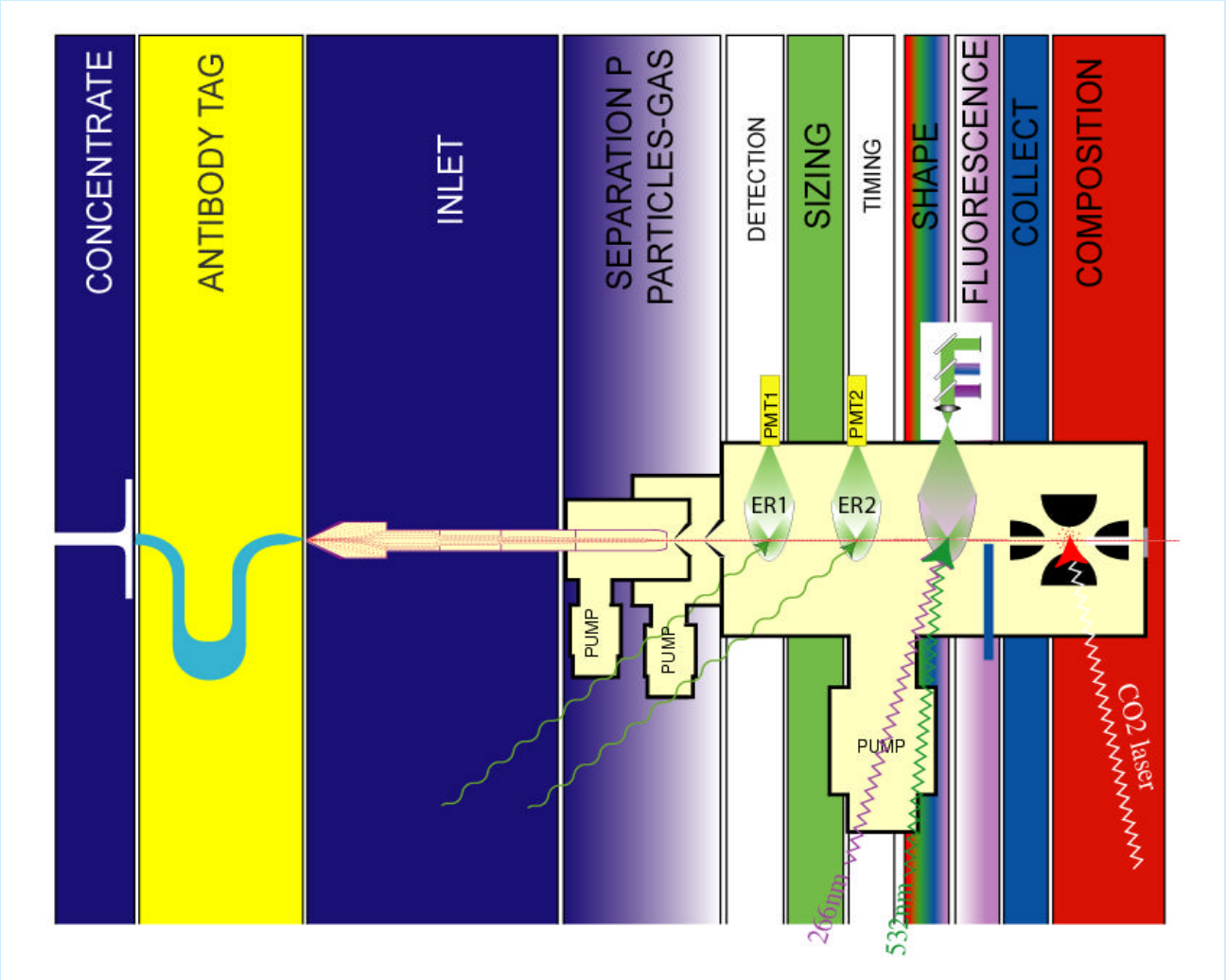
ESTIMATED SENSITIVITY FOR
SINGLE PARTICLE MASS SPECTROMETER

~1 org./ cm^3 second

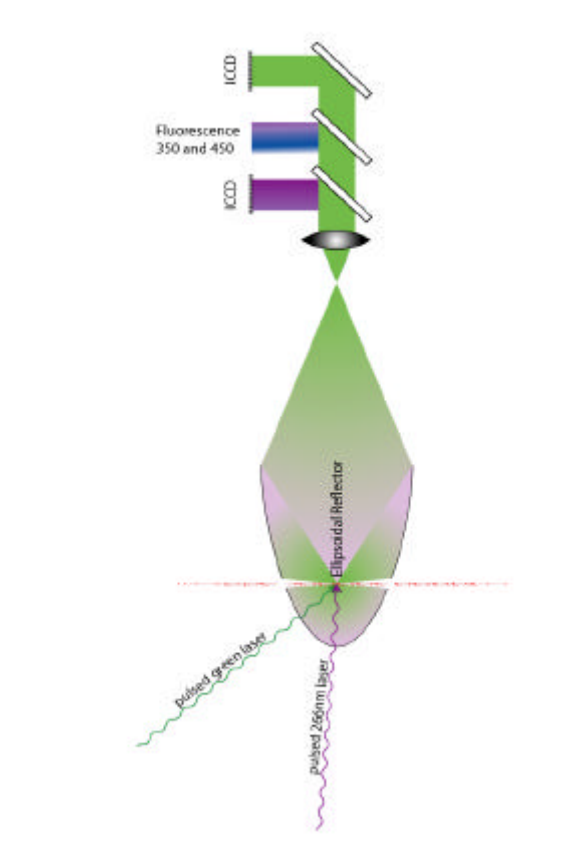
SINGLE SPORE ANALYSIS

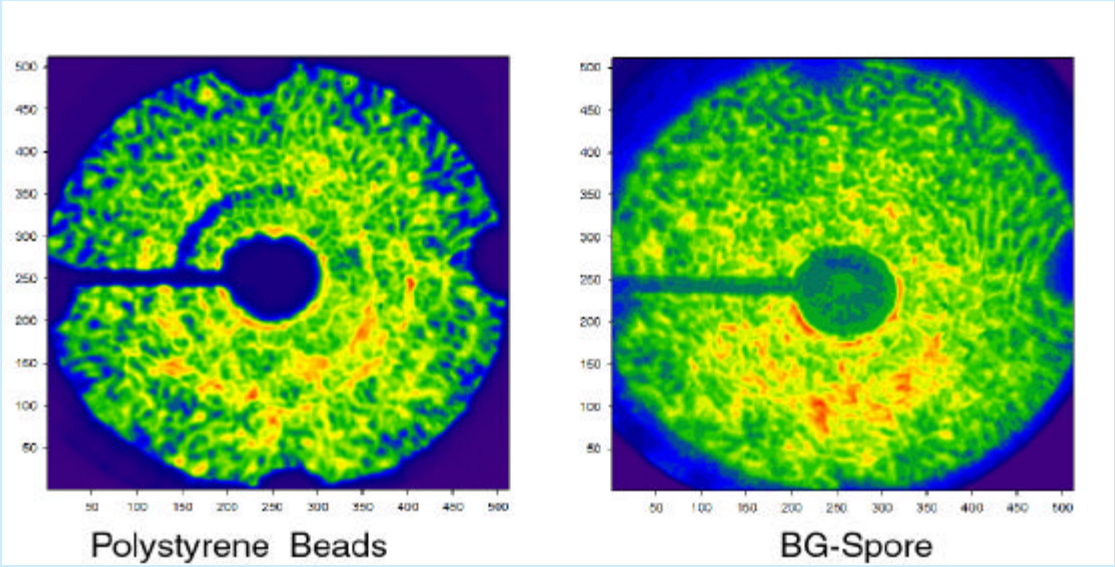
- Maximum sensitivity
- Zero background
- Stepwise identification and discrimination on the basis of:
  - Size
  - Shape
  - Bio-fluorescence
  - Mass spectral signature
  - Antibody reactivity
  - Select purify and collect individual spores for microscopic, DNA, and other analysis

5-D CHARACTERIZATION

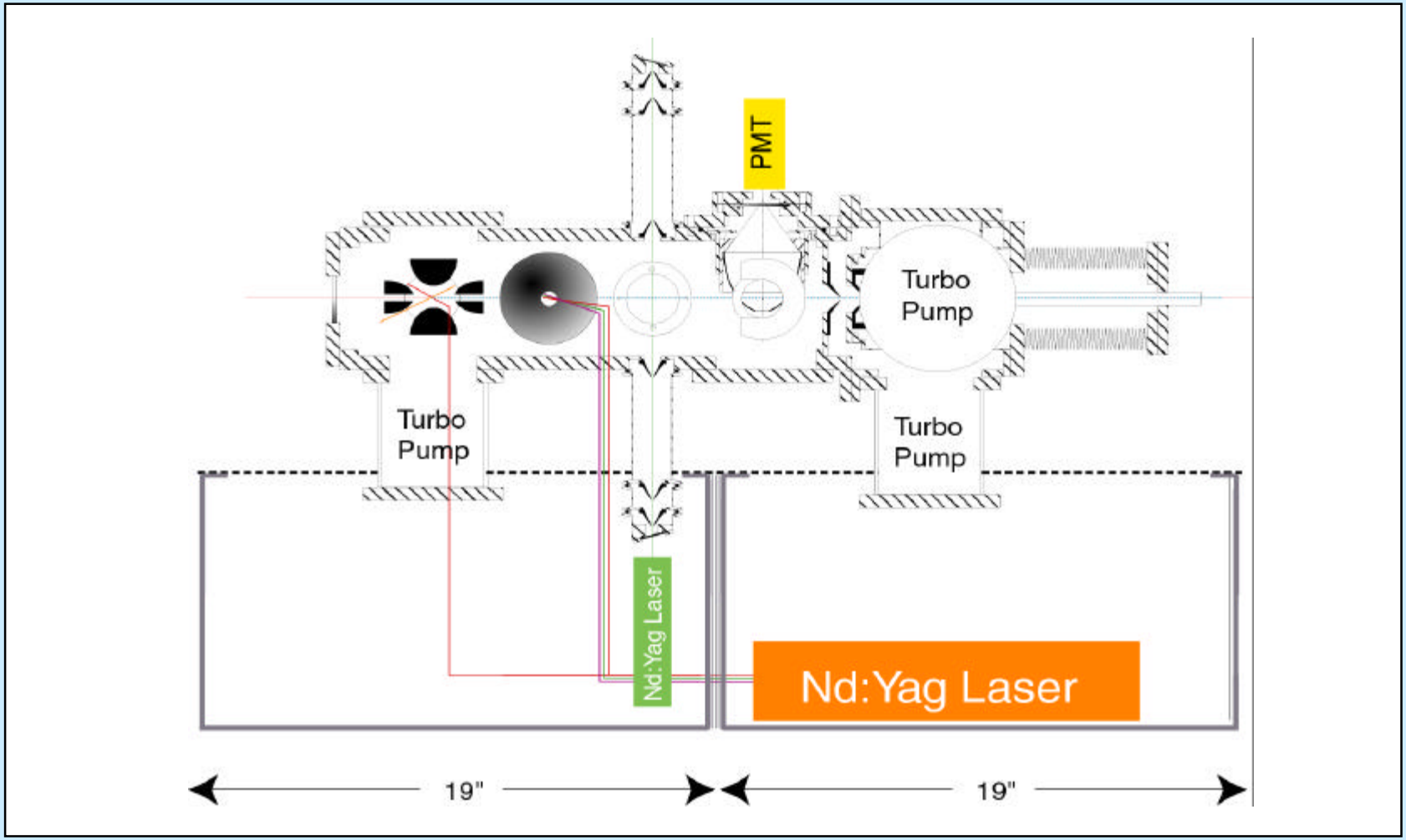


SHAPE & FLUORESCENCE





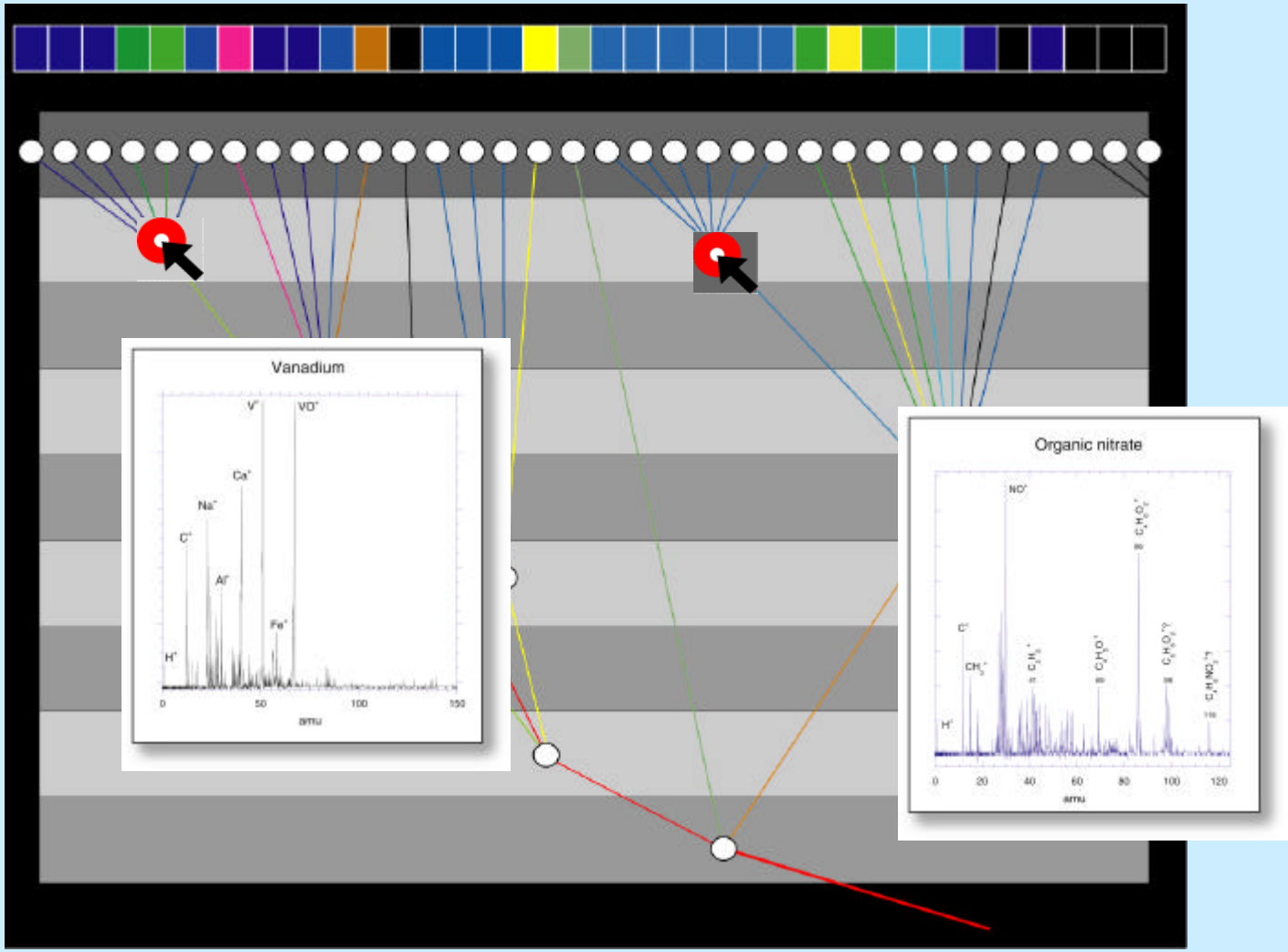
SCHEMATIC of a FIELD DEPLOYABLE INSTRUMENT



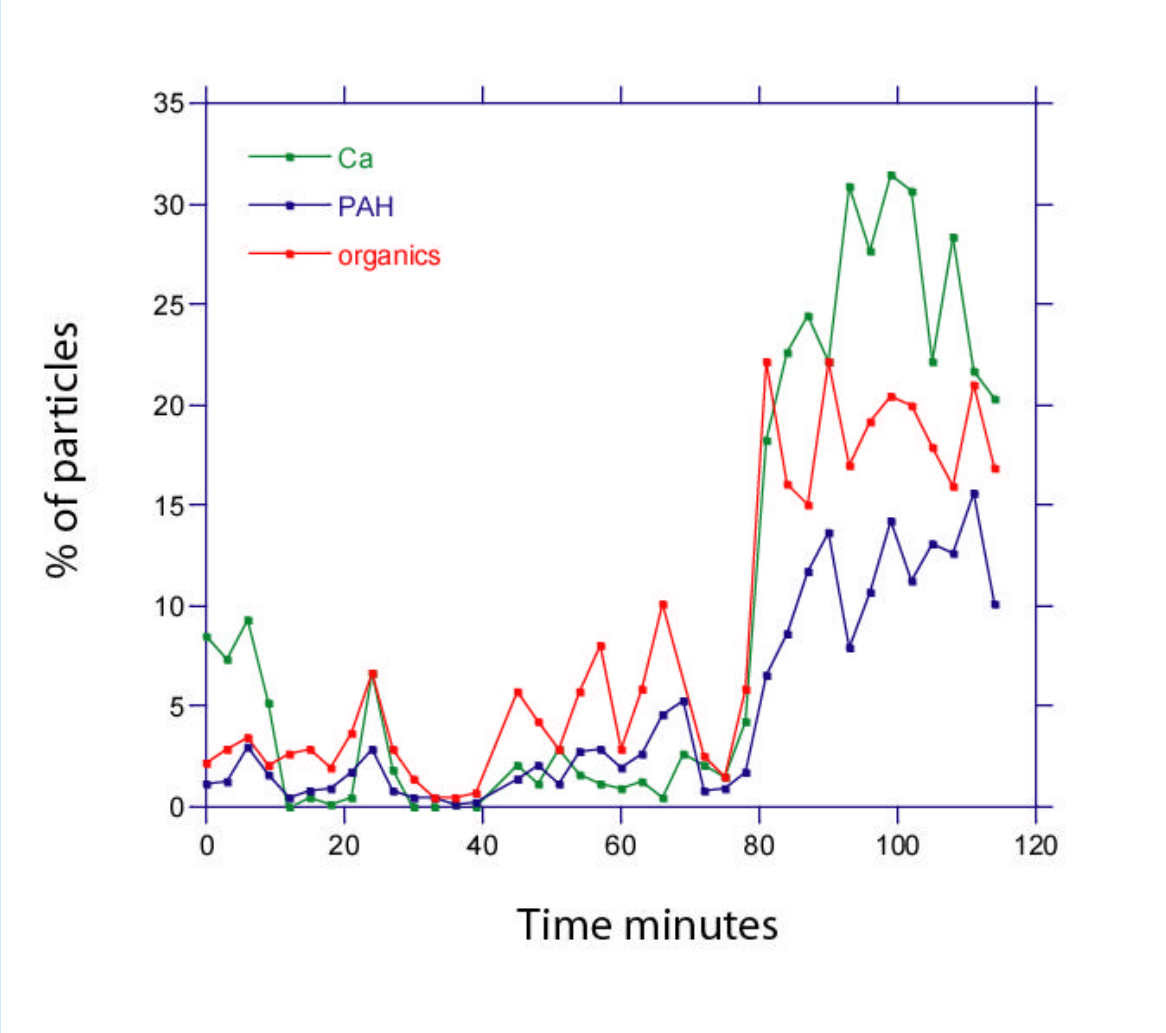
WHAT DO WE DO WITH ALL THE DATA?

- We can generate Gb of data each day.
- The data are detailed and if properly mined can provide insight into understanding aerosol sources and fate.
- So much information for such a little brain.
- We do not want to reduce (loose) the richness of the data.
- We cannot grow the brain
- We must develop tools that will make it possible to navigate through the data with ease.
- The tool must provide a multi-level view all the way from the individual particle to the entire data set with a road in-between.

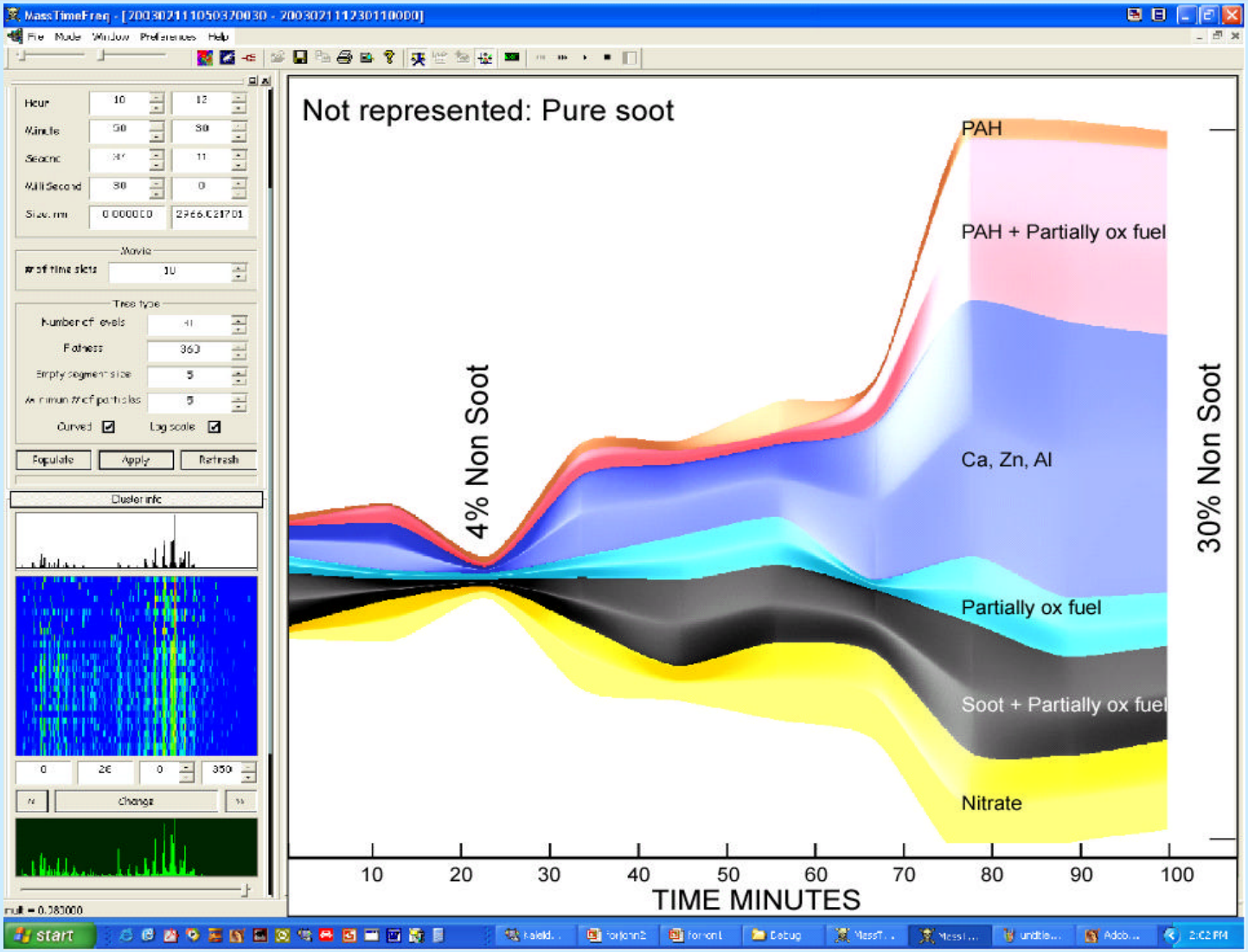
The Dendogram or Classification Tree



Composition Data with High Temporal Resolution



Data Mining with **SpectraMiner**



CONCLUSION

- Compact SPMS
- ~50 particles/sec
- 20nm to 3.5micron
- Size
- Composition by CI
- Optical properties
- Density
- Hygroscopicity
- Shape
- Fluorescence

- Real-time analysis and visualization
- Expert driven data classification
- Comprehensive data analysis and visualization of gases, MS, size distribution, etc.